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Towards Model Predictive Control: Online Predictions of Ammonium and Nitrate Removal by using a Stochastic ASM

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Abstract

Online Model Predictive Control of WRRF requires simple and fast models to improve the operation of energy-demanding processes, such as aeration for nitrogen removal. Selected elements of the ASM1 modelling framework for ammonium and nitrate removal were included in discretely observed Stochastic differential equations in which on-line data are assimilated to update the model states. This allows us to produce model based predictions including uncertainty in real time while it also reduces the number of parameters compared to many detailed models. It introduces only a small residual error when used to predict ammonium and nitrate concentrations in a small recirculating WRRF facility. The error when predicting 2 min ahead corresponds to the uncertainty from the sensors. When predicting 24 hours ahead the mean relative residual error increases to ~10% and ~20% for ammonium and nitrate concentrations, respectively. Consequently this is considered a first step towards stochastic model predictive control of the aeration process. Ultimately this can reduce electricity demand and cost for water resource recovery, allowing the prioritization of aeration in low electricity price periods.

Keywords

ASP, grey-box model, MPC, Prediction, Stochastic Differential Equations

INTRODUCTION

Mathematical modelling of Water Resource Recovery Facilities (WRRFs) is a widely established discipline for research, plant design, optimization, simulation of process control strategies, etc. For these purposes many models exist to choose between such as the Activated Sludge Models (ASM), the Anaerobic Digestion Models (ADM), the University of CapeTown (UCT) model or the TU Delft Phosphorous removal model (Henze et al., 2000; Gerneay et al. 2004; Batstone et al., 2002; Wentzel et al. 1992; Meijer, 2004; Hu et al. 2007). These complex models have differences in focus and as a result, in their structure. Hence choosing a model structure is, as with all modelling tasks, crucial to the outcome of the project. One important thing to include in the decision of a suitable model is the number of states and parameters. On one hand more states and parameters leads to a more detailed model. However, on the other hand more details introduce more inputs that need to be distinguished and therefore estimated, measured or, if this is not possible, guessed (Vanrolleghem et al. 1995). Furthermore numerically solving large models with many states leads to long simulation times which can be demanding for data-driven optimizations, which need to be run in short time intervals (seconds-minutes). Although not yet used in online operation of WRRFs, models can also be used to forecast future variables of interest for use in model predictive control (MPC), which means they should be fast and adaptable to online data.

The Activated Sludge Model number 1 (ASM1) (Henze et al. 1987) describes organic matter degradation, nitrification and denitrification in the activated sludge bioreactors. The model contains thirteen states variables and nineteen parameters. One of the most important challenges in using ASM1 in practice is arguably attributing the many stoichiometric and kinetic parameters (Gernay et al. 2004). The information needed for the characterization of these can come from three sources (Petersen et al. 2002): (1) default values from literature, (2) full-scale plant data such as those collected by online sensors, and (3) information obtained from lab-scale experiments. The type of data and calibration framework to use is highly dependent on the intended use (e.g. Petersen et al. 2002). While (1) might be good for educational purposes or comparison of control strategies (e.g. Gernaey et al., 2014), optimization of processes with respect to a specific plant requires (2) and/or (3) (Petersen et al. 2002).

MPC aims at predicting processes as a function of potential control actions and then choosing the best control scenario based on optimization of some objective function. In WRRFs this can translate to real-time modelling and forecasting of plant performance based on aeration control, optimizing electricity costs and effluent. When it comes to the selection of a suitable model for WRRF MPC strategies, the structure of states and parameters becomes particularly important. This is because of the following two reasons: firstly, because parameters should be statistically identifiable from online data to take proper advantage of the real-time setting and secondly, because the computational requirements should be sufficiently low to allow for real-time, recursive simulation of several control scenarios. This means, that a good online model should not have strong correlations between parameters, which is the case for parameters of ASM1 (Sharifi et al. 2014). Furthermore, the calibration should only depend on online data to avoid delay in updating the model, and hence the recalibration routine should not depend on information obtained from lab-scale experiments.

ASM1 has earlier been simplified to a linearized version to provide faster and yet reliable predictions (Smets et al. 2003). Furthermore ASM1 has been reduced in efforts to make more parsimonious models (e.g. Mulas et al. 2007; Cadet et al. 2014). However the focus of these models is not online operations, i.e. on being updated with online data only. Online model applications are here managed by the use of stochastic, Data-Driven Modeling (DDM) techniques. Many DDM methods exist depending on the purpose and data availability (e.g. Dürrenmatt and Gujer, 2012) and they are generally good alternatives when mechanistic models are not available or not valid (Gernaey et al. 2004). Since the detailed mechanistic understanding for the Activated Sludge Process (ASP) already exists, the use of DDMs would neglect all the already existing empirical process knowledge about nonlinearities and correlations.

Discretely observed Stochastic Differential Equation (SDE) based models are often referred to as stochastic “grey-box” (GB) models because the structure of the models represent both physical/chemical/biological, deterministic (“white-box”) understanding of the processes and statistical, stochastic (“black-box”) information indicated by data. Parameter calibration can be managed in the SDE-GB model by e.g. combining Extended Kalman Filtering (EKF) techniques and maximum likelihood estimation. This can be done statistically directly from online data by using e.g. the frameworks suggested by Kristensen et al. (2004), Tullekin (1993) or Jazwinsky (1970). Furthermore the EKF allows for optimal state estimation and handles additive noise effectively. 2012; Del Giudice et al. Carstensen (1994) concluded that in terms of process prediction and control, SDE-GB models of the wastewater processes perform significantly better than traditional black-box models like ARMAX models and also used them to statistically identify

Monod-kinetic parameters from online measurements in an Activated Sludge Process (ASP) (Carstensen et al. 1995). SDE-GB models have also been used to model incoming ammonium loads and first flush phenomena (Bechmann et al., 2000; Halvgaard et al. 2017), and to forecast rainfall-runoff flow and volume in sewer systems for use in real-time optimization (Thordarsson et al. 2015; Löwe et al., 2016).

In this paper we show that ASM1 can be rewritten to a simpler SDE-GB model that is applicable to online MPC purposes by treating state variables that show only slow and minor changes over short time horizons as model parameters that are kept fixed or intermittently re-estimated using online data. Thus, changes that occur slowly over weeks or months, such as changes in biomass, temperature, maintenance, wastewater composition etc., will be included in the parameters which are re-estimated intermittently with data from the past few days. The small error introduced by this simplification is estimated by a stochastic diffusion process and consequently it can be managed in the control setup. Following this methodology it is possible to create a Stochastic ASM with only three states representing ammonium concentration, nitrate concentration and available oxygen. This model can then be used to optimize the ammonium and nitrate removal process within a MPC approach.

This article presents a simple ASM based on SDEs, which uses flow and aeration data as input and assimilates on on-line measurements of ammonium and nitrate to update model states and thus prepare for providing the best possible forecasts at each time step. The model provides reliable online forecasts of the ammonium and nitrate removal process from a few minutes to up to 24 hours ahead and considers measurement errors. It is developed and tested with data from a small recirculation WRRF with alternating operation. The simplicity of the model makes it a general tool that can be useful on recirculation facilities with different configurations without changing the model setup.

CASE STUDY: NØRRE SNEDE WRRF

The model is developed and tested with data from Nørre Snede WRRF which is located in central Jutland, Denmark. The plant is designed to handle a maximum capacity of 9700 PE and the current load is approximately 4000 PE.

Operation and design

The WRRF includes several typical treatment processes, which the wastewater goes through before discharge. Listed in order from when the wastewater enters the process, these are pretreatment, grit removal and grease trap, chemical dosage, nitrification/denitrification and secondary treatment. The nitrification/denitrification in the Nørre Snede plant happens in a process tank with a total volume of 3500 m³. The tank is divided into three smaller chambers operated under different conditions. This is illustrated in Figure 1, which also shows that the aeration tank is equipped with nutrient sensors, aeration equipment, a recirculation pump and rotors which control the flow direction/velocity (direction shown with arrows in the figure, rotors are located at the bridge).

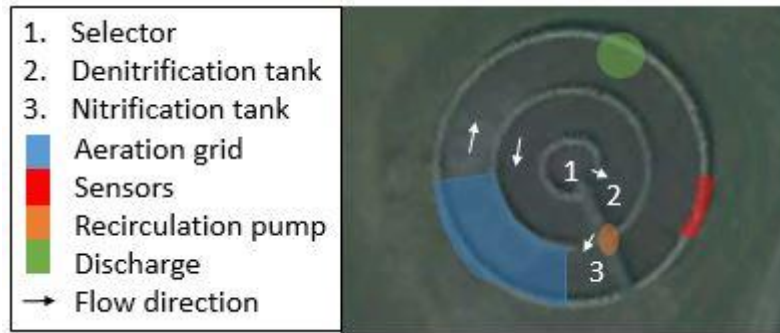


Figure 1. Overview of the process tank at Nørre Snede WRRF with important features marked.

The facility is currently operated with a Rule Based Control (RBC) strategy, as e.g. described by Isaacs & Thornberg (1998), Zhao et al. (2004) and Kim et al. (2014). In this case the control switches aeration on/off as a function of online ammonium and nitrate concentration measurements. Therefore the conditions are switching between anoxic and aerobic and the cycle lengths vary depending on the conditions in the process tanks. This is managed in the control platform STAR Utility SolutionsTM (Sørensen et al., 1994; Nielsen & Önnérth, 1995).

Data

The current control of the plant (i.e. actuator settings controlling aeration and inlet flow) is updated every two minutes and as result, aeration and inflow data are available every two minutes. The control rules are based on ammonium and nitrate signals, which are only sampled every five minutes directly in the aeration tank meaning that observations are sampled irregularly compared to control sampling. Calibration of sensors happens automatically 2-4 times per day, causing 30-60 minutes without new observations. There is a response time from when aeration starts/stops until this is observed by the sensors. This is due to hydraulics in the tank and processing time in the sensors (Rieger et al. 2003). This response time is estimated using the method suggested by Stentoft et al. (2017) where it is simply estimated as the time from conditions are shifting until a change in the trend in measurements is observed. Flow data are available at the outlet (after the settler) and is changing between 0 and ~45 m³/h because of a pumping scheme. To account for this scheme, flow data are filtered by a second order Fourier series. The available data used in this study is summarized in Table 1.

Table 1. Overview of online data used in this study. The uncertainty is based on the information available from the sensor manuals (HACH Lange Aps, 2013, 2014).

Symbol	Description	Sample frequency	Unit	Uncertainty
Q	Effluent Flow	2 min	m ³ /liter	Unknown
O	Actuator setting	2 min	mgO ₂ /liter	0
MsNH	Measured ammonium	5 min	mgN/liter	±3%
MsNO	Measured nitrate	5 min	mgN/liter	±5%

THEORY AND METHODOLOGY

In this section the model is identified. This includes a description of the SDE-GB model, a simplification of the ASM1 model with noise terms added, inclusion of aeration control and inflow as input. Last, the parameter estimation is briefly described.

Stochastic grey box model

A discretely observed stochastic greybox model can be written on state-space form as

$$\begin{aligned} dx_t &= f(x_t, u_t, t, \theta)dt + \sigma(u_t, t, \theta)d\omega \\ y_k &= h(x_k, u_k, t_k, \theta) + e_k \end{aligned}$$

where the description of the dynamics of the states x_t are divided into a (deterministic) drift term $f(x_t, u_t, t, \theta)dt$ and a (stochastic) diffusion term $\sigma(u_t, t, \theta)d\omega$. The system is observed only through y_k which is linked to x_t via the observation equation $h(x_k, u_k, t_k, \theta)$. The residual error is separated in to two terms. *Diffusion*, $\sigma(u_t, t, \theta)d\omega$ represents model approximations and undescribed noise disturbances, i.e. changes in biomass efficiency, unmodelled inflow, uncertainty of input variables (u_t), or true stochastic behaviour in the processes. *Measurement noise*, e_k represents the noise occurring due to imperfect accuracy of the measuring equipment, i.e. here measurement uncertainty in the ammonium and nitrate sensors.

Simplification of ASM1

Following the notation proposed by Corominas et al. (2010) the ordinary differential equations that govern ammonium, nitrate and oxygen in ASM1 can be written in a Gujer matrix as presented in Appendix together with a brief description of ASM1 parameters and state variables. The complexity of these equations is considered an obstacle for use in a real-time setting since many of the variables are unmeasured and consequently constants that will be difficult to distinguish. We therefore make simplifications to get a more suitable model. The main assumption in this simplification is that the model parameters will be re-estimated frequently, and therefore several state variables of ASM1 will become constant and some parameters will become unimportant.

- The rate, ρ_4 , which governs ammonification of soluble organic nitrogen can be neglected. This is considered reasonable as the ammonification rate parameter k_{am} is typically small compared to the process rates of nitrification and denitrification (Henze et al., 1987).
- The state variable S_B is constant during a day. In practice it will follow a diurnal pattern similar to that of S_{NH4} , but since S_B is not measured these will be difficult to distinguish.
- The state variables governing active heterotrophic and autotrophic biomasses X_{OHO} and X_{ANO} can be considered constant on a daily basis, and hence can be treated as parameters. This is considered reasonable as the biomass is known to only change over longer periods of time.
- The parameter for relative amount of N/COD in biomass, i_{N_COD} , can be neglected. A stoichiometric calculation by Henze et al. (1987) (assuming a typical cell formation, $C_5H_7O_2N$) indicate that i_{N_COD} is 0.086. This is very small compared to $1/Y_{ANO}$ which is approximately 4.2, and therefore it will be difficult to estimate.
- The half velocity parameters $K_{O2,OHO}$ and $K_{O2,ANO}$ for oxygen utilisation are considered equal ($K_{O2,OHO} = K_{O2,ANO} = K_{O2}$) as it is argued by Henze et al. (1987) that they are not, quantitatively, that different.

Applying these assumptions, the new, simple model of the ASP can be identified. The shorthand notation α_{NH_4} , α_{NO_3} and α_{O_2} to refer to these exact terms.

$$\begin{aligned} S'_{NH_4} &\approx \alpha_{NH_4} = -\theta_1 \left(\frac{S_{NH_4}}{K_{NH_4,ANO} + S_{NH_4}} \right) S_{O,MO} \\ S'_{NO_3} &\approx \alpha_{NO_3} = \theta_1 \left(\frac{S_{NH_4}}{K_{NH_4,ANO} + S_{NH_4}} \right) S_{O,MO} - \theta_2 \left(\frac{S_{NO_3}}{K_{NO_3,OHO} + S_{NO_3}} \right) (1 - S_{O,MO}) \\ S'_{O,MO} &\approx \alpha_{O_2} = - \left(\theta_3 + \theta_4 \left(\frac{S_{NH_4}}{K_{CNH_4,ANO} + S_{NH_4}} \right) \right) S_{O,MO} \end{aligned}$$

The half saturation constant $K_{CNH_4,ANO}$ is introduced because the state $S_{O,MO}$ is the Monod term indicating how quickly the process is running relative to the max rate i.e.

$$S_{O,MO} = \left(\frac{S_{O_2}}{K_O + S_{O_2}} \right)$$

The new seven parameters to estimate online are therefore θ_i , $K_{NO_3,OHO}$, $K_{NH_4,ANO}$ and $K_{CNH_4,ANO}$ where θ_i relate to the original ASM1 parameters as

$$\begin{aligned} \theta_1 &= \frac{1}{Y_{ANO}} \mu_{ANO,Max} X_{ANO} \\ \theta_2 &= \frac{1 - Y_{OHO}}{2.86 Y_{OHO}} \mu_{OHO,Max} \left(\frac{S_B}{K_{S_B} + S_B} \right) \eta_{\mu_{OHO,Ax}} X_{OHO} \\ \theta_3 &= \frac{1 - Y_{OHO}}{Y_{OHO}} \mu_{OHO,Max} \left(\frac{S_B}{K_{S_B} + S_B} \right) X_{OHO} C_1 \\ \theta_4 &= \frac{4.57 - Y_{ANO}}{Y_{ANO}} \mu_{ANO,Max} X_{ANO} C_2 \end{aligned}$$

Where C_1 and C_2 are correction factors that are introduced because $S_{MO,O}$ is the relative amount of oxygen.

Aeration control and inflow

For the purpose of using the model for MPC of N-removal, it is necessary to include the effect of aeration and incoming wastewater as external inputs in the model. The signal determining the intensity of aeration and measurements of incoming wastewater flow are available online and consequently the control should be a function of these i.e. $C_-(O, Q)$ is a function that describe the effect of inflow and aeration control on the given state. These functions are here determined from literature. More specifically, the two films theory (Lewis and Whitman, 1924) and diurnal variations in ammonium concentration and constant (low) nitrate concentrations in the incoming wastewater (Henze and Comeau, 2008). This means, that $C_{NH_4}(O, Q)$ and $C_{NO_3}(O, Q)$ are given as

$$\begin{aligned} C_{NH_4}(O, Q) &= (r_c + \rho Q) (\mu_{NH_4,in} + \sum_{i=1}^{n=2} [s_i \sin(iwt) + c_i \cos(iwt)]) - S_{NH_4} \\ C_{NO_3}(O, Q) &= (r_c + \rho Q) (\mu_{NO_3,in} - S_{NO_3}) \end{aligned}$$

Where $\mu_{NH_4,in}$, $\mu_{NO_3,in}$, s_i and c_i are parameters related to the inflow. Note that $\mu_{NO_3,in}$ is typically ~ 0 (e.g. Henze and Comeau, 2008). The parameters r_c and ρ are related to the recirculation (see Figure 1) to and the volume of the aeration tank. The control of the aeration is given as

$$C_{O,MO}(O, Q) = k_1 O (S_{O,MOmax} - S_{O,MO})$$

Where k_1 is a transfer constant (Lewis and Whitman, 1924) related to the size and efficiency of the aeration equipment. The maximum value of the relative oxygen state is 1, and hence $S_{O,MOmax}$ is set to 1 and should not be estimated.

Stochastic ASM

A 3-state greybox model governing the ammonium and nitrate concentrations in the aeration tank can be written as

$$dS_{NH_4} = f_{NH_4}(\cdot)dt + \sigma(u_t, t, \theta)d\omega_1 = \alpha_{NH_4}dt + C_{NH_4}(O_t, Q_t)dt + \sigma_{11}d\omega_1$$

$$dS_{NO_3} = f_{NO_3}(\cdot)dt + \sigma(u_t, t, \theta)d\omega_2 = \alpha_{NO_3}dt + C_{NO_3}(O_t, Q_t)dt + \sigma_{22}d\omega_2$$

$$dS_{O,MO} = f_{O,MO}(\cdot)dt + \sigma(u_t, t, \theta)d\omega_3 = \alpha_{O_2}dt + C_{O,MO}(O_t, Q_t)dt + \sigma_{33}d\omega_3$$

Where the deterministic terms α and C governs the ASP, the aeration and the inflow as described in previous sections. To avoid negative noise and to make estimation of small noise processes easier, the diffusion terms are estimated as exponential parameters (i.e. $\sigma_{ii} = \exp(s_{ii})$, $i \in [1,2,3]$). The system is discretely observed through ammonium and nitrate sensors in the aeration tank. The measurements ($MsNH$ and $MsNO$) from these relate to the system as

$$MsNH = S_{NH_4} + \exp(s_{1,NH_4})\epsilon_{NH_4}$$

$$MsNO = S_{NO_3} + \exp(s_{1,NO_3})\epsilon_{NO_3}$$

Where ϵ_{NH_4} and ϵ_{NO_3} are i.i.d. $\mathcal{N}(0, 1)$, i.e. the residuals of the measurements are normally distributed with zero mean and $\exp(s_{1,NH_4})$, $\exp(s_{2,NO_3})$ standard deviation. The changes in the states dS_{NH_4} , dS_{NO_3} and $dS_{MO,O}$ are given as state variables where ω_1 , ω_2 and ω_3 are 1-dimensional standard Wiener processes and $\exp(s_{11})$, $\exp(s_{22})$ and $\exp(s_{33})$ represent the deviation of these processes.

Online parameter Estimation in Stochastic ASM

The presented stochastic model fits the general model structure for continuous-discrete stochastic state space models, i.e. a model of the state variables in continuous time and measurements of some of the states at discrete times. The R-package CTSM-R (Juhl et al., 2016; Kristensen et al., 2004) can manage just this kind of system, and is therefore used to estimate parameters and predict the effect of control. This paper provides only a brief summary of how the package works and how it is used here. For further information on this, see CTSM-R (2018).

The parameter estimates are based on a maximum likelihood method, by assuming Gaussian distributed conditional probability densities.

$$L(\theta; Y_N) = \prod_{t=1}^N \frac{\exp(-0.5 \epsilon_t^T R_{t|t-1}^{-1} \epsilon_t)}{\sqrt{\det(R_{t|t-1}) 2\pi}} p(y_0|\theta)$$

where $\epsilon_t = y_t - \hat{y}_{t|t-1}$ ($\hat{y}_{t|t-1} = E(y_t|y_{t-1}, \theta)$) and $R_{t|t-1} = V(y_t|y_{t-1}, \theta)$. ϵ_t and $R_{t|t-1}$ are computed by means of a version of the Extended Kalman Filter (EKF) (e.g. Jazwinski, 1970). The likelihood function can be simplified to a simpler log-likelihood function by conditioning on y_0 and taking the negative logarithm. However this rewriting is omitted here. The parameter estimates are then obtained by minimizing this log-likelihood.

The mentioned EKF is a continuous-discrete time version of the EKF. With initial conditions for the model values and variance estimate ($\hat{x}_{1|0}$ and $P_{1|0}$) the filter approximations of the output predictions are given as

$$\begin{aligned}\hat{y}_{k|k-1} &= h(\hat{x}_{k|k-1}, u_k, t_k, \theta) \\ R_{k|k-1} &= C P_{k|k-1} C^T + S_k\end{aligned}$$

which here translates to

$$\begin{aligned}\hat{y}_{k|k-1} &= \begin{cases} \hat{S}_{NH_4 k|k-1} \\ \hat{S}_{NO_3 k|k-1} \end{cases} \\ R_{k|k-1} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} s_{1,NH_4} & 0 \\ 0 & s_{1,NO_3} \end{bmatrix} = \begin{bmatrix} p_{11} + s_{1,NH_4} & p_{12} \\ p_{21} & p_{22} + s_{1,NO_3} \end{bmatrix}\end{aligned}$$

Here C is the Jacobian of the observation equation, h . The innovation given by

$$\epsilon_k = y_k - \hat{y}_{k|k-1}$$

The Kalman gain, K_k , for the EKF is then calculated as

$$K_k = P_{k|k-1} C_k^T (R_{k|k-1})^{-1}$$

and the system is updated

$$\begin{aligned}\hat{x}_{k|k} &= \hat{x}_{k|k-1} + K_k \epsilon_k \\ P_{k|k} &= P_{k|k-1} - K_k R_{k|k-1} K_k^T\end{aligned}$$

\hat{x} is here the state estimates (S_{NH_4} , S_{NO_3} and $S_{O,MO}$). The state prediction is done numerically by

$$\begin{aligned}\frac{d\hat{x}_{t|k}}{dt} &= f(\hat{x}_{k|k-1}, u_t, t, \theta), t \in [t_k, t_{k+1}] \\ \frac{dP_{t|k}}{dt} &= A(t)P_{t|k} + P_{t|k}A(t)^T + \sigma(t)\sigma(t)^T, t \in [t_k, t_{k+1}]\end{aligned}$$

where $A(t)$ is the Jacobian of the drift term $f_i(t, \dots)$. This Jacobian is calculated using a method based on Speelpenning (1980). In calculations of the Jacobian it is assumed that $x = \hat{x}_{k|k-1}$, $u = u_k$, $t = t_k$ and the parameters, θ , are known. The ODEs are solved by numerical integration schemes suggested by Hindmarch (1983) (cited in Kristensen and Madsen, 2003, p. 17). This is to ensure an

intelligent re-evaluation of A and σ . From this construction we see, that the approximation is only good when nonlinearities are not too strong.

The estimation setup implies that initial state and parameter estimates are necessary in the parameter estimation procedure. These can be supplied either as prior distributions or simply just as estimates with some max and min boundaries. For most parameters these initial estimates are based on literature (e.g. Henze et al. 1987; Henze and Comeau 2008). However a few parameters are unnecessary or unable to be estimated. The initial state values $S_{NH4,0}$, $S_{NO3,0}$ and $S_{O,MO,0}$ can easily be estimated directly from data, as ammonium and nitrate are directly measured and oxygen signal is known, and hence these are considered unnecessary to estimate. Furthermore the parameters $K_{NO3,OH0}$, θ_3 and θ_4 are showing very small deviations and notably correlation with other parameters. It is also argued by Henze et al. (1987) that $K_{NO3,OH0}$ does not need estimation. For these reasons these are here kept constant at $[K_{NO3,OH0}, \theta_3, \theta_4] = [3.0, 5.0E-6, 1.0]$ and thereby reducing the amount of parameters to estimate.

RESULTS AND DISCUSSION

Firstly the model is qualitatively evaluated by comparing the model predictions with data and discussing parameter estimates. Secondly, the model is quantitatively evaluated by running it for 1 month and discussing statistics of residuals. We stress that the model is run “online” in the sense that parameters are estimated only by minimizing the objective function described in the previous section. Furthermore, the states S_{NH4} , S_{NO3} and $S_{O,MO}$, are updated using the EKF whenever a new measurement becomes available. Figure 2 shows an example of one prediction of ammonium given, inlet flow and aeration signal. The state, S_{NH4} , is updated with present data and then predicted two hours ahead. Clearly, uncertainty increases with increasing forecast horizon.

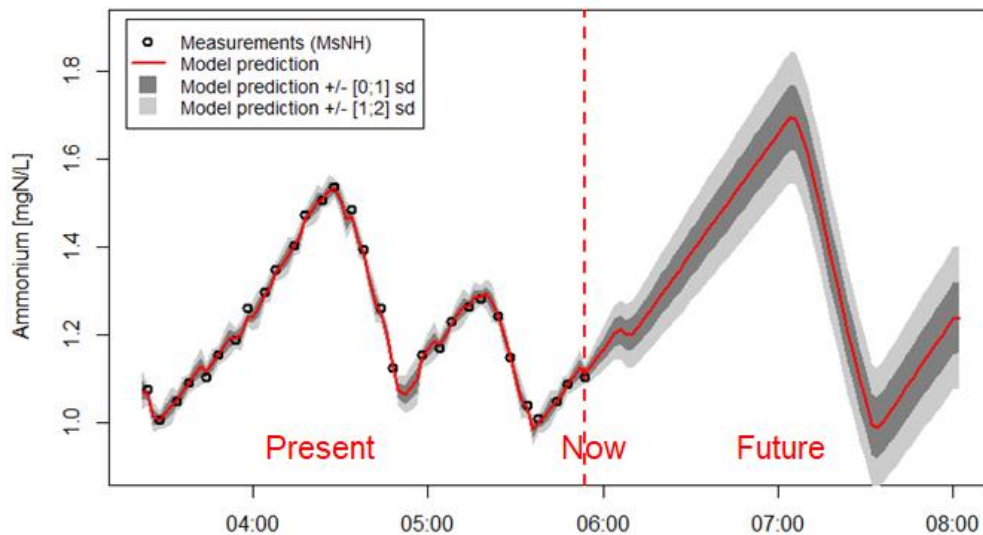


Figure 2. An example of a 2-hour prediction of ammonium concentrations (which is run every 2 minutes in the online set-up). The uncertainty increases the longer we look in the future, as estimated by the SDE.

Model dynamics

Parameters are estimated with data from a period in the beginning of October (2016) chosen arbitrarily among periods without rain. The length of the parameter estimation period is 4 days and 4 hours (corresponding to 3000 time steps of 2 minutes). These parameters are used to predict the concentrations of ammonium and nitrate in the aeration tank. Figure 3 and 4 show predictions of the ASP 60 time steps ahead corresponding to 2 hours, given the aeration signal. This is done for 24 hours, meaning that each time a new measurement becomes available a prediction similar to Figure 2 is made and compared with data. This is done during normal operation of the plant i.e. no rain and no (known) problems. .

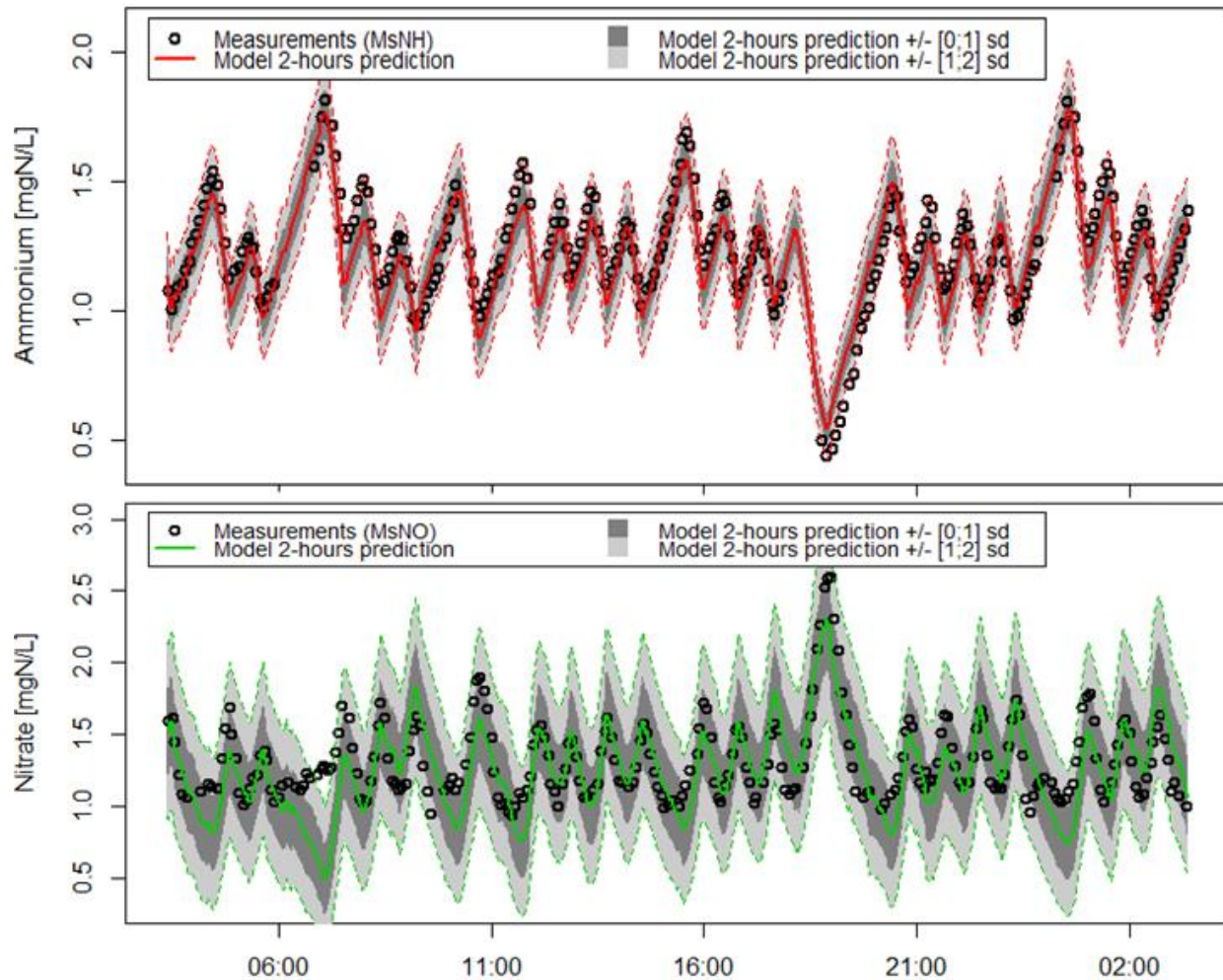


Figure 3. 2-hour predictions (60 timesteps of 2 mins) of the ammonium concentration in the aeration tank (S_{NH4}) with measured concentration (upper) and of the nitrate concentration in the aeration tank (S_{NO3}) with measured concentration (lower). Note that the y-axis differs because there is more variation in the nitrate observations.

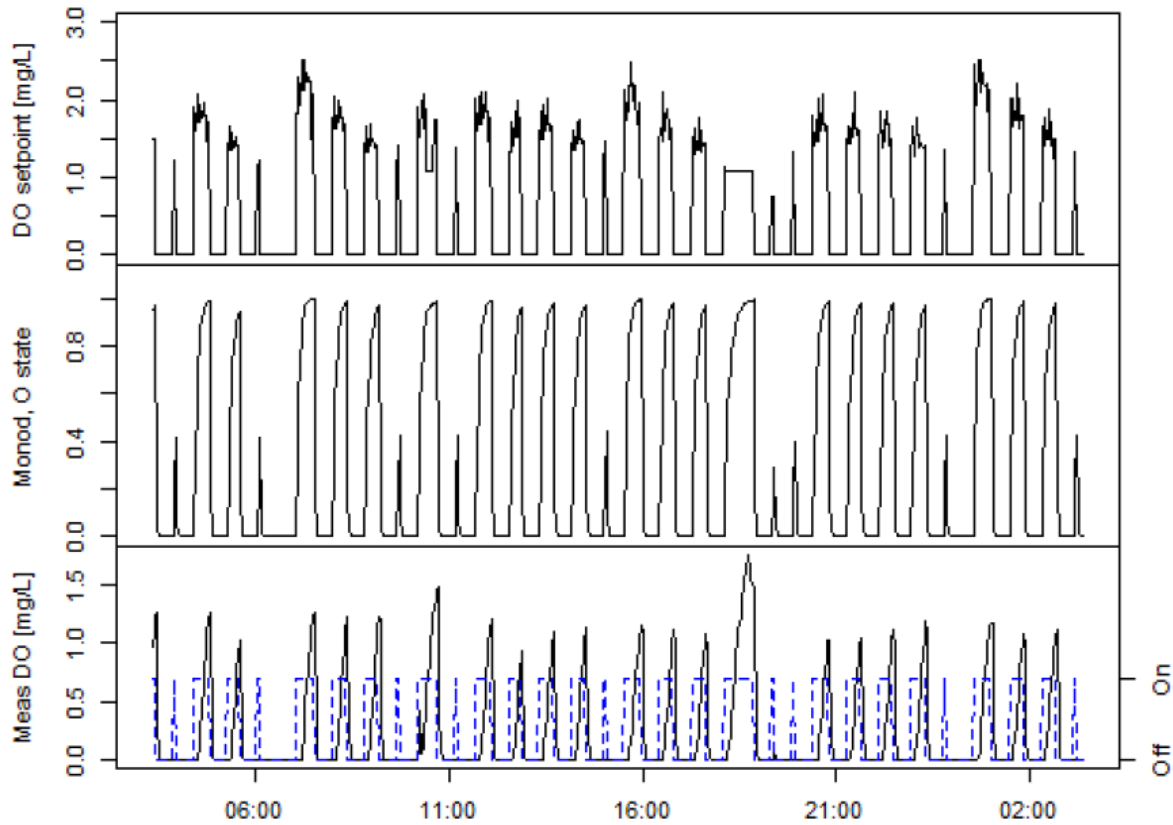


Figure 4. Upper: The input, O. Middle: the estimated Monod oxygen state, $S_{O,MO}$. Bottom: the measured oxygen in the aeration tank (black) and the binary signal for aeration on/off (blue).

In Figure 3 it is evident that under normal operation, the modeled ammonium concentration follows the same dynamics as the data. During the aeration phase the ammonium concentration decreases, and when aeration is switched off, NH_4 increases. In periods when no new data are received (i.e. calibration of the ammonium sensor from 17:30 to 18:30), the model continues to provide reliable estimates. The nitrate concentrations estimated in Figure 3 also follow dynamics similar to those in the data. It is noted that when aeration is off, nitrate decreases and when it is on, it increases. However, some dynamic starting at 06:00 does not follow the behavior shown by the sensor measurements. This period contains a relatively long timespan without aeration which will normally mean denitrification, however in this case we see that nitrate increases. This could be due to some unmodelled dynamics, problems with a drifting nitrate sensor or a large unusual load of nitrate in the influent coming from e.g. industry. Overall, the results show that the uncertainty of the nitrate predictions is greater than the uncertainty on ammonium predictions, and hence larger deviations from the modeled concentrations are expected. Figure 4 shows the estimates of the unmeasured state, $S_{O,MO}$. It is plotted together with the measured dissolved oxygen (DO) concentrations and the setpoint of the actuator, O. It is clear, that when the setpoint is lower, it takes a longer time for $S_{O,MO}$ to reach maximum level. The comparison between the aeration status and the measured oxygen concentrations highlight that short periods of aeration are not registered in measurements. This is caused by the location of the sensor, which is located opposite of the aeration grid (see Figure 1). This supports the choice of not including the measured DO as input/state in the model. Therefore

the actuator signal is considered superior as it reports all periods of added oxygen and furthermore it does not have any response time from when air is added until it is observed in the tank.

Parameter Estimates

The parameters that are estimated in the before mentioned period are presented in Table 2.

Table 2. Parameter estimates and standard deviations. Parameters are calculated using 3000 timesteps of data corresponding to 4 days and 4 hours. The period is from beginning of October 2016.

Parameter	Estimate	Standard deviation
Simplified ASM		
$K_{NH_4,ANO} [mgN/L]$	4.80E-01	1.80E-01
$K_{CNH_4,ANO} [mgN/L]$	1.05E-03	6.99E-04
$\theta_1 [mgN/L]$	5.00E-02	5.39E-03
$\theta_2 [mgN/L]$	2.47E-01	1.59E-02
Aeration control and inflow		
$s_1 [mgN/L]$	1.14E+00	6.63E-01
$s_2 [mgN/L]$	-5.63E-01	3.73E-01
$c_1 [mgN/L]$	4.25E-01	3.24E-01
$c_2 [mgN/L]$	-5.82E-02	1.75E-01
$\mu_{NH_4,in} [mgN/L]$	1.35E+01	6.76E+00
$\mu_{NO_3,in} [mgN/L]$	1.10E-02	2.01E-02
$K_1 [L/mgO]$	1.12E-01	6.48E-03
$\rho []$	1.08E-05	1.64E-05
$r_c []$	7.21E-04	4.31E-04
Noise and diffusion terms		
$s_{11} [\log(mgN/L)]$	-4.79E+00	7.65E-02
$s_{22} [\log(mgN/L)]$	-3.20E+00	2.06E-02
$s_{33} []$	-2.86E+00	2.16E-01
$s_{1,NH} [\log(mgN/L)]$	-8.66E+00	1.26E-01
$s_{1,NO} [\log(mgN/L)]$	-1.80E+01	2.56E+01

Some parameters are difficult to evaluate as these represent some catchment/plant specific information. Nonetheless, parameters are here discussed and in some cases compared with literature:

- The residual errors (which are split into diffusion and measurement noise) are found to be similar to what is estimated for ammonium in the aeration tank by Halvgaard et al. 2017 in another plant with similar sensors and configuration. However the uncertainty on the measuring equipment is much smaller compared to what is informed by the sensor manufacturer (see Table 1).
- The Monod kinetics parameter, $K_{NH_4,ANO}$, is found to be similar to what is statistically estimated by Carstensen et al. 1995. Here it was found to be between 0.44 and 0.76 among

different plants and catchments. It is though lower than ~ 1 which is suggested by Henze et al. 1987.

- The mean incoming concentrations of ammonium, $\mu_{NH_4, in}$ and nitrate, $\mu_{NO_3, in}$ seem reasonable as these are similar to what is typically found in a “catchment with little industrial activity” according to Henze and Comeau, 2008. The diurnal variations in ammonium, s_1 , s_2 , c_1 and c_2 are catchment specific. However these are considered reasonable as they produce a variation that is comparable with the one presented in Henze and Comeau (2008) i.e. similar shape with peaks in the morning and afternoon.
- The new parameters θ_1 and θ_2 are difficult to compare with literature as these depend on many parameters and the states X_{ANO} and X_{OHO} . However following the typical parameter suggestions from Henze et al. 1987, these should be $3.33 X_{ANO}$ and $0.82 X_{OHO}$ respectively.
- The parameters related to the incoming water, r_c and ρ , are estimated to $7.21E-04$ and $1.08E-5$ respectively. Summing these and multiplying the mean flow with ρ we get $1.11E-3$. This is slightly more than the expected $3.43E-4$ which is found by dividing mean flow with the volume of the process tank. This difference can be due to the recirculation which happens between the nitrification and denitrification tanks.
- The relative oxygen transfer rate k_1 depends on many factors such as tank design (e.g. reactor geometry, aeration design), physico-chemical properties (e.g. liquid composition, viscosity, temperature) and the presence of biomass (e.g. Pittoir et al., 2014). Therefore it is difficult to determine empirically as it varies between facilities and over time.

Model Performance

The models predictive ability is tested by re-estimating parameters every 1 hour for a period of 1 month and 1 week, starting late September (2016). The model is then used to predict concentrations of ammonium and nitrate 1, 60 and 720 time steps ahead (corresponding to 2 min, 2 hours and 1 day, respectively). The predictions are compared with data and a 24 hour running mean absolute residual is calculated. Figure 5 illustrates how this changes over time for predictions 2 hours ahead (60 time steps). Table 3 shows the statistics of the mean absolute residual for all the different prediction horizons.

In Figure 5 it is evident that during some periods (i.e. October 2nd, October 15th and October 22nd) the uncertainty increases. Comparing with rain data supplied by the Danish Meteorological Institute (DMI, 2018) it is seen that many of these periods are characterized by wet weather. This is also indicated in Table 3 where the general picture is that uncertainty increases during wet weather. In Table 3 it is also seen that the relative 2 min uncertainty is $\sim 2\%$ for ammonium and $\sim 6\%$ for nitrate. This is comparable with the sensor uncertainty listed in Table 1 and indicates that the 2 min predictions cannot be further improved even with a more detailed deterministic model. The 2 hours and 24 hours predictions perform worse than the sensor uncertainty. This can on one hand indicate that there is room for improvement, but can on the other hand also mean that there is some stochastic behavior (e.g. incoming nutrients or biomass efficiency) which is more pronounced when predicting further ahead from the EKF state update. It should be added that the treatment requirements for Nørre Snede WRRF govern that during a 24 hours period, the ammonium concentration should be < 2 mgN/L and total N should be < 8 mgN/L in the outlet. Consequently this means that accurately predicting ammonium is more important because nitrate only effects on

total N. The relative uncertainties on ammonium and nitrate of <10% and <20% respectively (in dry weather, 24 hours ahead) are considered sufficient for stochastic model predictive control.

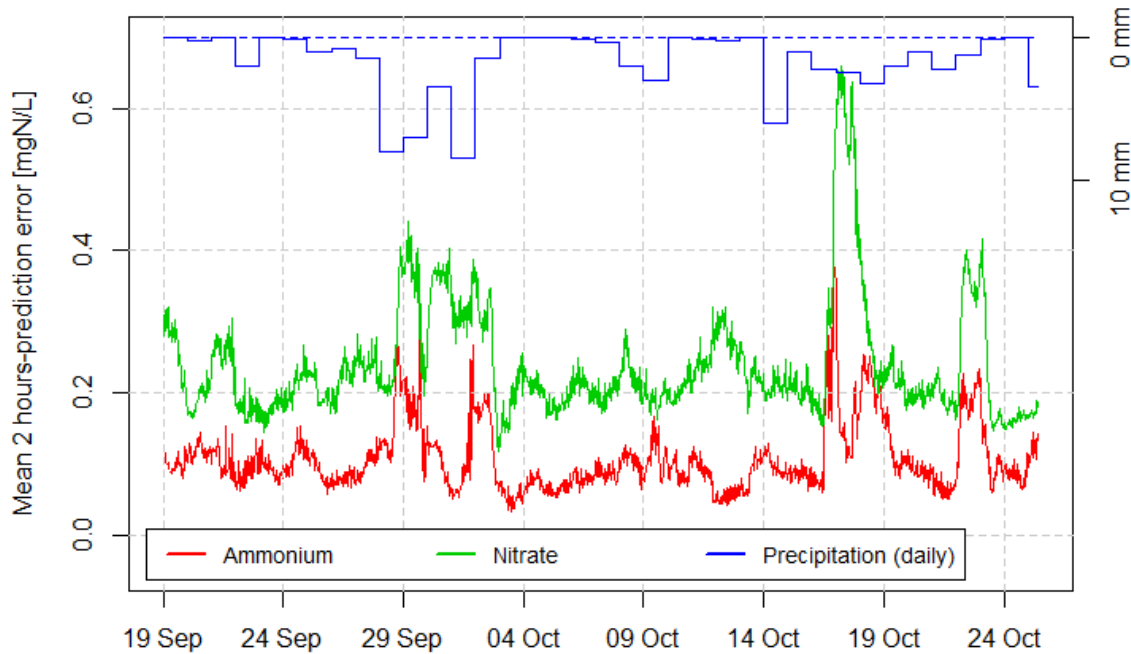


Figure 5. Mean absolute error for 2 hours (60 timesteps of 2 mins) prediction of ammonium and nitrate. Plotted with daily precipitation data from DMI (2018).

Table 3. Summary statistics of the residuals of the model predictions, based on residuals gained from using the model with data from Nørre Snede WRRF for a period of 1 month in September/October 2016. “Precipitation” indicates whether only dry weather periods are considered (no) or all periods (Yes).

Precipitation*	Prediction	Mean absolute error [mgN/L]		Relative absolute error [-]	
		No	Yes	No	Yes
Ammonium	2 min	0.0264	0.0278	0.0212	0.0223
	2 hours	0.0884	0.1065	0.0709	0.0855
	24 hours	0.0925	0.129	0.0855	0.104
Nitrate	2 min	0.0804	0.081	0.0594	0.0598
	2 hours	0.212	0.2399	0.157	0.177
	24 hours	0.246	0.374	0.1815	0.276

*Wet weather periods are the following periods 28 Sep - 02 Oct, 15 Oct - 19 Oct and 22 Oct – 23 Oct.

Towards Model Predictive Control - simplified and full ASM models

The results in Table 3 are difficult to compare with full ASM models, as to our knowledge there exist no framework for making the full ASM models online adaptive to data. However, our results can be compared with data-driven model parameter estimations of full ASMs (i.e. other methods

that rely only on data from online ammonium/nitrate sensors). One example of such an approach is provided by Sin et al. (2008), where the parameters of an ASM2d model were estimated using only frequently sampled online ammonium, nitrate and oxygen measurements (sampled every 5 minutes, similar to this study) in the 50.000 PE Haaren WRRF in the Netherlands with alternating control of aeration. Parameters were calibrated using Monte-Carlo simulations to minimize a weighted sum of squared errors (WSSE) based on a calibration period of 16.117 measurements (56 days). Model performance was compared with data in a validation period of 9.217 measurements (32 days). The results showed a Mean Absolute Error (MAE) for ammonium of 1.39 mgN/l and 0.98 mgN/l in the calibration and validation periods, respectively. For nitrate concentrations a MAE of 2.56 mgN/l and 2.31 mgN/l were found. These error values are 10 times larger than what we have found in this study, cf. Figure 3. Also, the framework presented in Sin et al. (2008) differs from this study in as the model states are not updated when new data becomes available and hence short time predictions in the validation period (up to 24 hours ahead) are not based on all the information available in an on-line situation. Additionally it is noted that the framework by Sin et al. (2008) required some computation time (45 min per simulation (in 2008) on a PC, and 500 Monte Carlo simulations where used to obtain a model), which makes it non-ideal for online applications.

The development of tools for online performance optimization of WRRFs using models is crucial for exploiting the full potential of digitalization. Hence, the development of robust approaches to online identifiable ASMs for improved short horizon predictions is needed. These models should also include additional processes such as biological removal of COD and P, for achieving an overall improvement of all the removal processes in the plant. This paper provides a first step in this direction with online predictions of ammonium and nitrogen removal.

CONCLUSION

Grey box models based on stochastic differential equations are efficient tools as they can estimate both processes and noise from real time data. Here a stochastic model of an aeration tank is proposed. The model contains a deterministic term consisting of both a simplified ASM and input functions determining the influence of control and inflow. The model is used to predict the nitrification/denitrification in Nørre Snede WRRF in Denmark as a function of aeration and inflow.

The results show that despite the simple structure of the proposed model, the dynamics of the nutrient concentrations are captured. Quantitative investigation show that the processes are predicted accurately, i.e. 24 hour predictions of the ammonium and nitrate concentrations in the aeration tank are predicted with relative errors of <10% and <20% respectively. Consequently this is considered a step towards stochastic model predictive control of water resource recovery processes.

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REFERENCES

- Batstone, D. J., Keller, J., Angelidaki, R. I., Kalyuzhnyi, S. V., Pavlostathis, S. G., Rozzi, A., Sanders, W. T. M., Siegrist, H. & Vavilin V. A. (2002) Anaerobic Digestion Model No. 1. Scientific and Technical Report No 13. IWA Publishing, London, UK. Connelly, N. G., Damhus, Bechmann H., Madsen H., Kjølstad Poulsen N. & Nielsen M. K., (2000) Grey Box Modelling of First Flush and Incoming Wastewater at a wastewater treatment plant, *Environmetrics* 2000(11): 1-12
 Cadet, C. (2014). Simplifications of Activated Sludge Model with preservation of its dynamic accuracy. In IFAC.
 Carstensen J., Harremoës P. & Madsen H., (1995). Statistical Identification of Monod-Kinetic Parameters From On-line Measurements. *Wat. Sci. Tech.* 31(2): 125-133
 Carstensen J., (1994) Identification of Wastewater Treatment Processes, PhD thesis, IMSOR, Technical University of Denmark
 Corominas, L. L., L. Rieger, I. Takács, G. Ekama, H. Hauduc, P. A. Vanrolleghem, Oehmen, A., K. V. Gernaey, M. C. M. van Loosdrecht, and Y. Comeau. 2010. New framework for standardized notation in wastewater treatment modelling. *Water Science and Technology* 61 (4): 841–857
 CTSM-R, 2018, CTSM-R – Continuous Time Stochastic Modelling for R, <http://ctsm.info>, visited January 31st 2018
 DMI., (2018), Vejrkarkiv, <https://www.dmi.dk/vejr/arkiver/vejrkarkiv/> - visited January 17th 2018
 Del Giudice, D., Lowe, R., Madsen, H., Mikkelsen, P. S., and Rieckermann, J. (2015). Comparison of two stochastic techniques for reliable urban runoff prediction by modeling systematic errors. *Water Resources Research*, 51(7):5004–5022.
 Dürrenmatt, D., & Gujer, W. (2012). Data-driven modeling approaches to support wastewater treatment plant operation. *Environmental Modelling & Software*, 30, 47–56. <http://dx.doi.org/10.1016/j.envsoft.2011.11.007>.
 Gernaey, K. V., Jeppsson, U., Vanrolleghem, P. A., Copp, J. B. (2014) *Benchmarking of Control Strategies for Wastewater Treatment Plants*, Scientific and Technical Report Series, IWA Publishing Company, London, United Kingdom
 Gernaey, K. V., van Loosdrecht, M. C. M., Henze, M., Lind, M., and Jorgensen, S. B. (2004). Activated sludge wastewater treatment plant modelling and simulation: state of the art. *Environmental Modelling and Software*, 19(9):763–783.
 HACH Lange APS (2013). Amtax sc, Amtax indoor sc Brugsanvisning. HACH Lange APS, 8a edition.
 HACH Lange APS (2014). Nitratax sc - Betjeningsvejledninger. HACH Lange APS, 6a edition.
 Halvgaard, R. F., Vezzaro, L., Grum, M., Munk-Nielsen, T., Tychsen, P., & Madsen, H. (2017). Stochastic Greybox Modeling for Control of an Alternating Activated Sludge Process. DTU Compute. (DTU Compute-Technical Report-2017, Vol. 08).
 Henze, M. and Comeau, Y. (2008). Biological Wastewater Treatment: Principles Modelling and Design - Chapter 3, Wastewater Characterization. IWA Publishing, London.
 Henze, M., Gujer, W., Mino, T. & van Loosdrecht, M. C. M. 2000 Activated Sludge Models: ASM1, ASM2, ASM2d and ASM3. Scientific and Technical Report no 9. IWA Publishing, London, UK.
 Henze, M., Jr, C. P. L. G., Gujer, W., Marais, G. v. R., and Matsuo, T. (1987). Activated Sludge Model no. 1. Technical report, IAWPRC.
 Hindmarch, A. C. (1983). ODEPACK, A Systematized Collection of ODE Solvers in: "Scientific Computing (IMACS Transaction on Scientific Computation)". Amsterdam, 1st edition.
 Hu, Z., Wentzel, M. C. & Ekama, G. A. 2007 A general kinetic model for biological nutrient removal activated sludge systems: model development. *Biotechnol. Bioeng.* 98(6), 1242–1258.
 Isaacs S. H. & Thornberg D., (1998). A comparison between model and rule based control of a periodic activated sludge process, *Water Science and Technology* 37 (12): 343–351
 Lewis, W. and Whitman, W. (1924). Principles of Gas Absorption. *Industrial and Engineering Chemistry*, 16(12):1215–1220.
 Löwe, R., Vezzaro, L., Mikkelsen, P.S., Grum, M., Madsen, H. (2016): Probabilistic runoff volume forecasting in risk-based optimization for RTC of urban drainage systems. *Environmental Modelling and Software*, **80**, 143-158.
 Jazwinski, A. H. (1970). Stochastic Processes and Filtering Theory. Academic Press.
 Juhl R., Møller J.K., Jørgensen J.B., Madsen H. (2016) Modeling and Prediction Using Stochastic Differential Equations. In: Kirchsteiger H., Jørgensen J., Renard E., del Re L. (eds) Prediction Methods for Blood Glucose Concentration. Lecture Notes in Bioengineering. Springer, Cham
 Kim H., Kim Y., Kim M., Piao W., Gee J. & Kim C., (2014) Performance Evaluation of a Full-scale Advanced Phase isolation ditch Process by Using Real-time Control Strategies, *Korean J. Chem. Eng.*, 31(4): 611-618
 Kristensen, N. R., Madsen, H., and Jørgensen, S. B. (2004). Parameter estimation in stochastic grey-box models. *Automatica*, 40(2):225–237
 Kristensen, N. R. and Madsen, H. (2003). Continuous Time Stochastic Modelling Mathematics Guide.

- Meijer, S. C. F. 2004 Theoretical and Practical Aspects of Modelling Activated Sludge Processes. PhD Thesis. Delft University of Technology, The Netherlands.
- Mulas M., Tronci S. & Baratti R., (2007) Development of a 4-Measureable States Activated Sludge Process Model Deduced from the ASM1, IFAC Proceedings vol. 1, June 4-6 Cancún, Mexico
- Nielsen M.K. and Önnérth T.B., (1995), Improvement of a recirculating plant by introducing STAR control, *Water Science & Technology*, Volume 31(2), 171 – 180
- Petersen B., Vanrolleghem P. A., Gernaey K & Henze M., (2002) Evaluation of an ASM1 model calibration procedure on a municipal-industrial wastewater treatment plant, *Journal of Hydroinformatics*. Volume 4(1): 15-38
- Pittoors E., Guo Y. & Van Hulle S. W. H., (2014), Modeling Dissolved Oxygen Concentration for Optimizing Aeration Systems and Reducing Oxygen Consumption in Activated Sludge Processes: A Review, *Chem. Eng. Comm.*, 201: 983-1002
- Rieger, L., Alex, J., Winkler, S., Boehler, M., Thomann, M. & Siegrist, H. (2003) Progress in sensor technology - progress in process control? Part 1: Sensor property investigation and classification. *Water Science and Technology* 47 (2), 103–112
- Sin G., De Pauw D. J.W., Weijers S., & Vanrolleghem P., (2008) An efficient approach to automate the manual trial and error calibration of activated sludge models, *Biotechnology and Bioengineering*, volume 100 (3): 516-528
- Sharifi S., Murthy S., Takács I., & Massoudieh A., (2014) Probabilistic parameter estimation of activated sludge processes using Markov Chain Monte Carlo. *Water Research*. Volume 50:254-266
- Smets I.Y., J.V. Haegebaert, R. Carrette, J.F. Van Impe (2003). Linearization of the activated sludge model ASM1 for fast and reliable predictions. *Water Res.* **37**, 1831-51
- Stentoft P. A., Munk-Nielsen T., Mikkelsen P. S. and Madsen H., (2017). A Stochastic Method to Manage Delay and Missing Values for In-Situ Sensors in an Alternating Activated Sludge, in *Proceedings of ICA 2017 11-14 June 2017 in Québec City, Québec, Canada*
- Sørensen, J., Thornberg, D.E., and Nielsen, M.K. (1994). Optimization of a Nitrogen-Removing Biological Wastewater Treatment Plant Using On-Line Measurements. *Water Environment Research*, 66(3), 236–242.
- Thordarson, F., Breinholt, A., Moller, J. K., Mikkelsen, P. S., Grum, M., and Madsen, H. (2012). Evaluation of probabilistic flow predictions in sewer systems using grey box models and a skill score criterion. *Stochastic Environmental Research and Risk Assessment*, 26(8):1151–1166.
- Tullekin H. J. A. F., (1993) Grey-box Modelling and Identification Using Physical Knowledge and Bayesian Techniques, *Automatica*, 29(2): 285-308
- Vanrolleghem P. A., Van Daele, M. & Dochain D. (1995). Structural Identifiability of Biokinetic Models of Activated-Sludge Respiration. *Water Research*, 29(11), 2571–2578. [https://doi.org/10.1016/0043-1354\(95\)00106-U](https://doi.org/10.1016/0043-1354(95)00106-U), 10.1016/0043-1354(95)00106-U
- Wentzel, M. C., Ekama, G. A. & Marais, G. v. R. 1992 Process and modelling of nitrification denitrification biological excess phosphorus removal systems—a review. *Water Sci. Technol.* 25(6), 59–82.
- Zhao, H., Freed, A.J., Dimassimo, R.W., Hong, S.N., Bundgaard, E., and Thomsen, H.A. (2004). Demonstration of Phase Length Control of BioDenipho Process Using On-line Ammonia and Nitrate Analyzers at Three Full-Scale Wastewater Treatment Plants. *WEFTEC*.

APPENDIX

The ordinary differential equations that govern ammonium, nitrate and oxygen in ASM1 (Henze et al. 1987) are presented in a Gujer matrix in Table A using notation proposed by Corrominas et al. (2010). The parameters and state variables in this matrix are briefly specified in Table B.

Table A. Gujer matrix for selected ASM1 equations.

Process	Rate	S_{NH_4}	S_{NO_3}	S_{O_2}
Aerobic growth of heterotrophs	$\mu_{OHO,Max} \left(\frac{S_B}{K_{S_B} + S_B} \right) \left(\frac{S_{O_2}}{K_{O_2,OHO} + S_{O_2}} \right) X_{OHO}$	$-i_{N_COD}$		$-\frac{1 - Y_{OHO}}{Y_{OHO}}$
Anoxic growth of heterotrophs	$\mu_{OHO,Max} \left(\frac{S_B}{K_{S_B} + S_B} \right) \left(\frac{K_{O_2,OHO}}{K_{O_2,OHO} + S_{O_2}} \right) \left(\frac{S_{NO_3}}{K_{NO_3,OHO} + S_{NO_3}} \right) \eta_{\mu_{OHO,Ax}} X_{OHO}$	$-i_{N_COD}$	$-\frac{1 - Y_{OHO}}{2.86 Y_{OHO}}$	
Aerobic growth of autotrophs	$\mu_{ANO,Max} \left(\frac{S_{NH_4}}{K_{NH_4,ANO} + S_{NH_4}} \right) \left(\frac{S_{O_2}}{K_{O_2,ANO} + S_{O_2}} \right) X_{ANO}$	$-i_{N_COD} - Y_{ANO}^{-1}$	Y_{ANO}^{-1}	$-\frac{4.57 - Y_{ANO}}{Y_{ANO}}$
Ammonification of soluble organic nitrogen	$k_{am} S_{B,Org,N} X_{OHO}$	1		

Table B. A brief description of selected parameters and state variables of ASM1.

Notation	Description
Parameters	
$\mu_{OHO,Max}$	Monod maximum heterotroph growth
$\mu_{ANO,Max}$	Monod maximum autotroph growth
Y_{OHO}	Heterotrophic yield
Y_{ANO}	Autotrophic yield
$K_{O_2,ANO}$	Oxygen half saturation coefficient for autotrophs
$K_{O_2,OHO}$	Oxygen half saturation coefficient for heterotrophs
$K_{NO_3,OHO}$	Nitrate and nitrite half-saturation coefficient for heterotrophs
$K_{NH_4,ANO}$	Ammonium and ammonia half-saturation coefficient for autotrophs
K_{S_B}	Half saturation coefficient for heterotrophic biomass
k_{am}	Ammonification rate
i_{N_COD}	Mass of nitrogen relative to mass COD in products from biomass
$\eta_{\mu_{OHO,Ax}}$	Correction factor for anoxic growth of heterotrophs
State variables	
S_B	Readily biodegradable Substrate
S_{O_2}	Oxygen (negative COD)
S_{NO_3}	Nitrate and nitrite nitrogen
S_{NH_4}	Ammonium and ammonia nitrogen
$S_{B,Org,N}$	Soluble biodegradable organic nitrogen
X_{OHO}	Active heterotrophic biomass
X_{ANO}	Active autotrophic biomass